ADVANCED BURN-RATE MODELING AND COMBUSTION DIAGNOSTICS FOR NEW, ROCKET-MISSILE AND GUN PROPELLANTS

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SUMMARY

Advanced, burn-rate, propellant modeling is critical for developing new rocket-missile and gun propellants for Future Combat Systems and for providing a fundamental screening tool that can result in substantial cost savings compared to missile and gun firings. In this summary, we report the detailed chemical kinetics and burn rate prediction of hexahydro-1,3,5-hexanitro-1,3,5-triazine (RDX) and selected high-energetic binders and nitrate esters.

Figure 1 shows a burning strand of RDX composite at ~15 atm (left) and a depiction of the molecular nature of the burning propellant with thermochemical and physical processes that illustrate the complexity of the overall process (right). We modeled the gas phase at a high level of detail and finessed the condensed phase by a semi-empirical approach. Our chemical mechanism consists of ~400 elementary reactions involving 100 species that we obtained from a critical literature review. We tested this mechanism with our burner flame apparatus: i.e. H_2, NH_3/N_2O, NO_2 flames for the N-H-O chemistry. Flame temperatures, as well as stable and radical species concentrations were measured by laser spectroscopy and molecular beam mass spectrometry, and then compared to those obtained with the SANDIA PREMIX flame code containing subsets of the detailed chemical mechanism. We also measured the rates of questionable reactions with our high-temperature kinetics apparatus or calculated them with quantum mechanic-based programs. The $NH+H_2$ and $NH+CO_2$ rates in the 400-1200K-temperature range will be presented at the meeting.

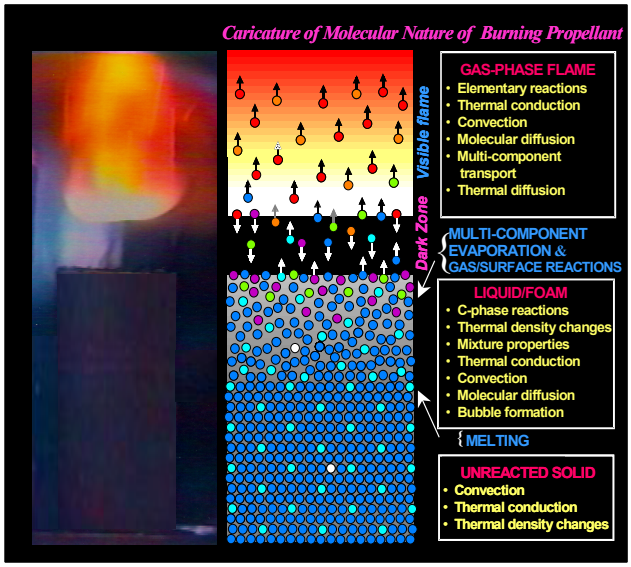

Fig 1. Burning RDX: Photograph (left) and molecular depiction (right).

The output of our burn-rate predictor is shown in Figures 2 and 3. Figure 2, which was generated with our in-house postprocessing program, shows a chemical pathway diagram focusing on the nitrogenous species of RDX burning at 1 atm. It reveals the decomposition channels of RDX and the intermediate and final products produced. All of the major and minor species, as well as most of the radical intermediates, are observed experimentally. Figure 3 shows the burning rate of RDX in the 1-100 atm range. Our model predicts well the observed

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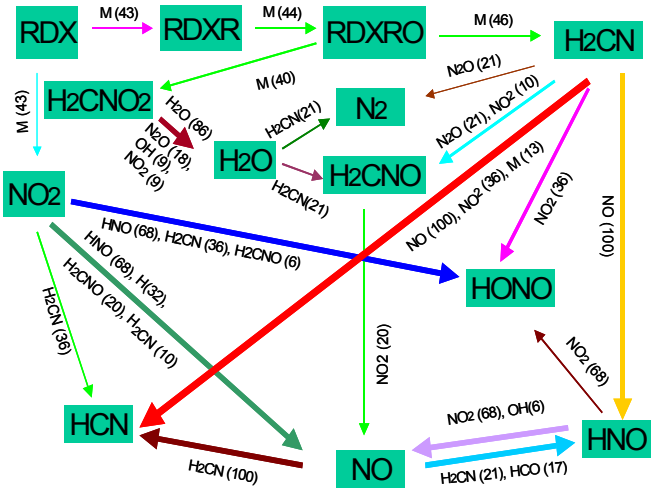

Fig. 2. RDX chemical pathway diagram obtained with our burn rate predictor.

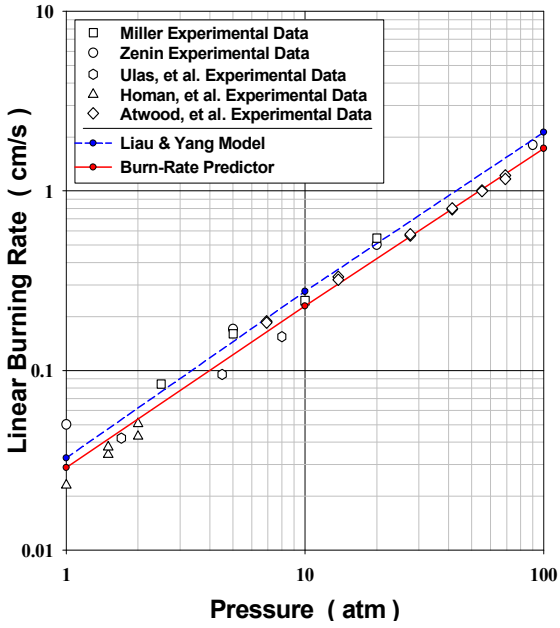

Fig. 3. Observed and calculated burn rate of RDX.

experimental data, as well as the modeled data by Liau and Yang.

Our advanced experimental and modeling capabilities provide the necessary tools for characterizing low-signature, insensitive, rocket-missile and gun propellants for energy-managed, military systems that require greater range and flexibility. We have developed a burn-rate model with detailed chemical kinetics for solid propellants, and presented our results for RDX. Our work on high-energy binder and nitrate esters is ongoing.